Isonipecotic acid, N-(2-fluoro-3-trifluoromethylbenzoyl)-, butyl ester

Inchi: InChI=1S/C18H21F4NO3/c1-2-3-11-26-17(25)12-7-9-23(10-8-12)16(24)13-5-4-6-14(15(1

InchiKey: MXUPELHLGHGJPZ-UHFFFAOYSA-N

Formula: C18H21F4NO3

SMILES: CCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2F)CC1

Mol. weight [g/mol]: 375.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.92		Crippen Method
logp	4.040		Crippen Method
mcvol	255.930	ml/mol	McGowan Method
rinpol	2332.00		NIST Webbook
rinpol	2332.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361309&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.